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## Article

# Simulation of Steam Gasification in a Fluidized Bed Reactor with Energy Self-Sufficient Condition

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**Abstract:** The biomass gasification process is widely accepted as a popular technology to produce fuel for the application in gas turbines and Organic Rankine Cycle (ORC). Chemical reactions of this process can be separated into three reaction zones: pyrolysis, combustion, and reduction. In this study, sensitivity analysis with respect to three input parameters (gasification temperature, equivalence ratio, and steam-to-biomass ratio) has been carried out to achieve energy self-sufficient conditions in a steam gasification process under the criteria that the carbon conversion efficiency must be more than 70%, and carbon dioxide gas is lower than 20%. Simulation models of the steam gasification process have been carried out by ASPEN Plus and validated with both experimental data and simulation results from Nikoo & Mahinpey (2008). Gasification temperature of 911 °C, equivalence ratio of 0.18, and a steam-to-biomass ratio of 1.78, are considered as an optimal operation point to achieve energy self-sufficient condition. This operating point gives the maximum of carbon conversion efficiency at 91.03%, and carbon dioxide gas at 15.18 volumetric percentages. In this study, life cycle assessment (LCA) is included to compare the environmental performance of conventional and energy self-sufficient gasification for steam biomass gasification.

**Keywords:** energy self-sufficient; fluidized bed gasifier; ASPEN Plus; life cycle assessment (LCA)

## 1. Introduction

With increasing energy demands of the world and environmental awareness, biomass gasification is an alternative technology to solve those problems. Moreover, this technology can significantly reduce the volume of biomass waste generated in developing societies [1]. Gasification is a thermo-chemical conversion which converts solid fuel such as biomass into useful synthesis gas (mixture of CO, H<sub>2</sub>, and CH<sub>4</sub>) through partial oxidation. It can be further processed to produce heat and electricity [2]. Several biomass-based power technologies are analyzed. Megwai and Richards [3] studied five power generation processes (gas turbines, steam turbines, micro gas turbines, Stirling engines, and internal combustion engines) in terms of electric performance, environmental indicators, and economic evaluations. The results showed that the internal combustion engine and the Stirling engine proved to be the most economically feasible for small-scale power production. However, the internal combustion engine power system emitted more NO compared with other systems. It was also indicated that additional costs might be incurred for installing gas cleaning systems for treating the synthetic gas.

A typical thermochemical process generally follows the chemical operation zones: drying, pyrolysis, combustion, and reduction. The biomass feedstock is firstly heated (dried) to remove some moisture, and then it undergoes a pyrolysis step to be decomposed at high temperature. The products of the pyrolysis step (i.e., solid, liquid, and gas) react among themselves as well as

with the gasifying medium to form the final gasification product. The chemical reactions that occur during the pyrolysis step and gasification step can be basically presented in Table 1. According to Sinha et al. [4], the pyrolysis region could be divided into three zones: an endothermic primary decomposition zone at  $T < 250\text{ }^{\circ}\text{C}$ ; an exothermic partial zone at  $250\text{ }^{\circ}\text{C} < T < 340\text{ }^{\circ}\text{C}$ ; and an endothermic surface char zone at  $340\text{ }^{\circ}\text{C} < T < 520\text{ }^{\circ}\text{C}$ . They concluded that the overall heat of reaction at higher heat fluxes was exothermic.

**Table 1.** Basic reactions in gasification of carbonaceous materials [5,6].

Reaction	Reaction Name	$\Delta H_{25\text{ }^{\circ}\text{C}}$ (kJ/mol)
<u>Pyrolysis</u>		
Biomass $\rightarrow$ Char + Tar + Volatiles	Pyrolysis reaction	
<u>Combustion</u>		
$\text{C} + 0.5\text{O}_2 \rightarrow \text{CO}$	Partial combustion reaction	−111
$\text{C} + \text{O}_2 \rightarrow \text{CO}_2$	Total combustion reaction	−394
$\text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2$	Carbon monoxide combustion reaction	−283
<u>Reduction</u>		
$\text{C} + \text{CO}_2 \rightarrow 2\text{CO}$	Boudouard reaction	+172
$\text{C} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{CO}$	Steam-carbon reaction	+131
$\text{C} + 2\text{H}_2 \rightarrow \text{CH}_4$	Hydrogasification	−74.8
$\text{CO} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{CO}_2$	Water-gas-shift reaction	−41.2
$\text{CO} + 3\text{H}_2 \rightarrow \text{CH}_4 + \text{H}_2\text{O}$	Methanation reaction	−206

Several models have been proposed in order to explain the gasification process, with an interest towards the design, simulation, optimization, and process analysis of gasifiers. The models can be divided into kinetic rate models and thermodynamic equilibrium models. The thermodynamic models, with independent with gasifier designs, are a useful tool for preliminary comparison and for process studies on the influence of the most important fuel and process parameters. However, thermodynamic models cannot give real results because they do not take into account time and specific material and equipment data. Kinetic rate models always contain parameters that limit their applicability to different plants, but they give real results [7]. A novel kinetic reaction model was presented by Peters et al. [8]. The model was implemented in ASPEN Plus. It was able to calculate yields and composition of the pyrolysis products of unknown lignocellulosic feedstock based on its biochemical composition with a minimum of input.

The use of carbon dioxide ( $\text{CO}_2$ ) as an oxidizing agent in biomass gasification has become a new frontier for the research on biomass conversion as well as  $\text{CO}_2$  utilization. The addition of  $\text{CO}_2$  in the gasification process shows many advantages such as greater synthesis gas yield [9]. Im-Orb et al. [10] studied two gasification processes with different gasifying agents (i.e., steam–air and steam- $\text{CO}_2$ ) and developed a thermodynamic gasification model using ASPEN Plus. Suitable conditions offering the highest amount of the synthesis gas with the desired  $\text{H}_2/\text{CO}$  ratio at thermal self-sufficient operation of the gasifier were determined. It was concluded that the steam- $\text{CO}_2$  system gave a higher synthesis gas productivity and lower  $\text{H}_2/\text{CO}$  ratio. However, for the aspect of total energy consumption, the steam–air system consumed less energy and thermal self-sufficient conditions could be achieved. Pfeifer et al. [11] modified the conventional dual fluidized bed gasification process with the absorption enhanced reforming (AER) process. The use of  $\text{CO}_2$ -adsorbing bed materials within dual fluidized bed gasifiers made a gas product with hydrogen content up to 75 vol. % available.

The types of a gasifier available for commercials include fixed bed, fluidized bed, and entrained flow. For large-scale applications, the most preferred and reliable system is the circulating fluidized bed. In contrast, the fixed bed system is more appropriate for a small-scale system [12]. Examples of steam gasification process studies are atmospheric fluidized bed combustor [13], biomass gasification in a fluidized bed reactor [14,15], steam blown dual fluidized bed gasification [16], and bubbling fluidized bed gasification [17]. Shehzad et al. [18] studied the thermodynamic performance of a municipal solid waste (MSW) gasification system with a circulating fluidized bed gasifier under various operating conditions. A computer simulation model was used in order to evaluate the exergetic efficiency of the

MSW to syngas conversion process for each individual unit. A water gas shift pilot plant employing a commercial Fe/Cr-based catalyst was operated with tar-rich product gas from the industrial scale and commercial biomass steam gasification plant in Oberwart, Austria. The volumetric CO content in the product gas was decreased to below 2%. Furthermore, a CO conversion of 92% was obtained [19]. Most studies have been focused on the effects of operating conditions in the gasification process without concern for the energy self-sufficiency in the steam gasification process. The advantages of an energy self-sufficient system can also be the minimum quantity of energy required, the maximum yields operating efficiency, and the minimum production time [20]. Therefore, the energy self-sufficiency of the steam gasification process is the focus in this research.

Recently, gasification models have been developed based on process simulator ASPEN Plus models combining thermodynamic and kinetic rate models in the gasification process. Nikoo & Mahinpey [14] developed a model based on ASPEN Plus with external FORTRAN subroutines for reaction hydrodynamics and kinetics to simulate the biomass gasification in a fluidized bed reactor. Different sets of operating conditions were used to demonstrate and validate the model. Mansaray et al. [21] proposed an ASPEN Plus model combining Gibbs equilibrium models to simulate rice husk gasification based on material balance, energy balance, and chemical equilibrium relations. Lui et al. [22] developed a biomass gasification model by considering thermodynamic equilibrium and ignoring the kinetic factors. The effects of gasification temperature, gasification pressure, and equivalence ratio (ER) on the gas component composition, gas yield, and gasification efficiency were studied using ASPEN Plus based on the Gibbs free energy minimization method. For the results, the optimal ER for gasification was approximately 0.3, and the gasification efficiency was 85.92%. Begum et al. [23] studied the gasification of three different biomass feed stocks (food waste (FW), municipal solid waste) via the ASPEN Plus software. The effects of operating parameters, such as temperature and equivalence ratio (ER) were investigated.

The objective of this study is to optimize the required energy in a steam gasification process by considering three operating parameters (gasification temperature, equivalence ratio, and steam-to-biomass ratio) in order to achieve an energy self-sufficient condition. The simulation model of the steam gasification process has been carried out by ASPEN Plus and validated with both experimental data and simulation results of Nikoo & Mahinpey [14]. Life cycle assessment (LCA) has been used as a tool to evaluate the environmental impacts associated with all stages of a process or a product. In this study, it is applied to provide environmental analysis of conventional and energy self-sufficient gasification of pine sawdust processes.

## 2. ASPEN Plus Model

### 2.1. Assumptions

Assumptions made in modeling the gasification process are as follows:

- The simulation process is run under a steady state condition.
- The operation zone inside the gasifier is an isothermal condition.
- The residence time for reactants is sufficiently high to reach the equilibrium of Gibbs free energy during pyrolysis reaction.
- The volatile products of biomass are mainly comprised of  $H_2$ , CO,  $CO_2$ ,  $CH_4$ , and  $H_2O$ .
- Char only contains carbon black and ash.
- The simulation is carried out with power-law kinetics.

### 2.2. Model Description

Operation steps of the gasification process in a fluidized bed reactor are separately considered in ASPEN Plus simulation: pyrolysis zone, combustion and reduction zone, and gas-solid separation. A series of various reactor blocks are properly selected and sequenced as shown in Figures 1 and 2.

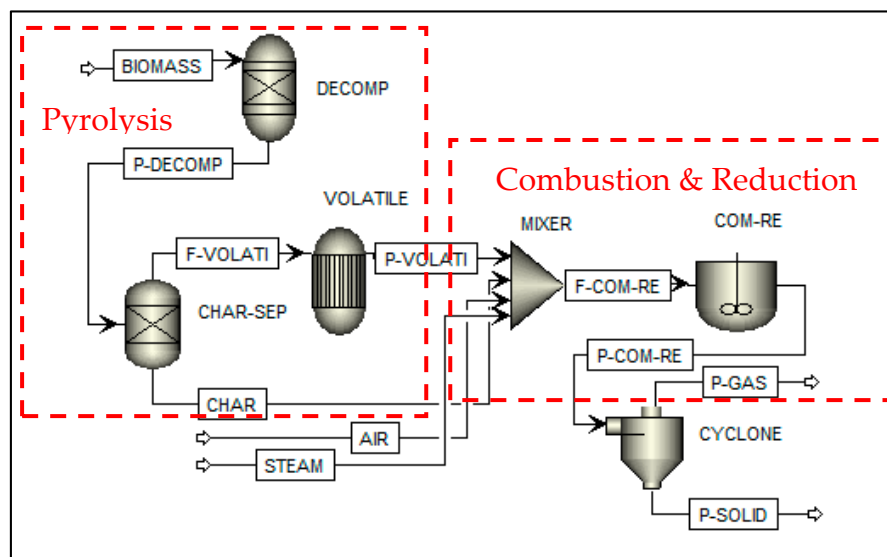


Figure 1. The schematic diagram of simulation model for the steam gasification process.

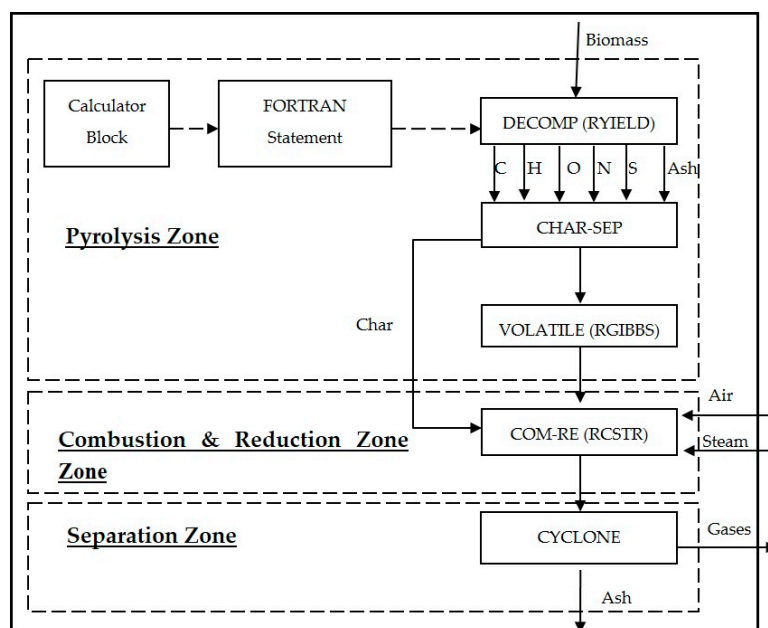


Figure 2. Simulation procedure of the steam gasification process.

The ASPEN Plus (Version 7.3, AspenTech, Burlington, MA, USA) yield reactor, RYIELD (model ID: DECOMP), is used to simulate the decomposition of the biomass feed stream. In this step, biomass is converted into its constituting components including carbon, hydrogen, oxygen, sulfur, nitrogen, and ash by specifying the yield distribution according to the biomass proximate and ultimate analysis.

The ASPEN Plus Gibbs reactor, RGIBBS (model ID: VOLATILE), is used for volatile reaction, in conformity with the assumption that volatile reactions follow the equilibrium of Gibbs free energy. Biomass consists of mainly C, H, O, N, S, ash, and moisture. Carbon partly constitutes the gas phase, which takes part in devolatilization, and the remaining carbon comprises part of the solid phase (char) and subsequently results in char gasification.

A separation module (model ID: CHAR-SEP) is used to separate the volatile materials and solids. It can separate the solid phase of carbon with the assumption that char is considered as only components of carbon black and ash.

The operating conditions including temperature, pressure, and possible production components are identified in the reactor VOLATILE. This reactor calculates the composition of product with the assumption that the residence time for reactants is sufficiently high to reach the equilibrium of Gibbs free energy during pyrolysis reaction.

The ASPEN PLUS CSTR reactor, RCSTR (model ID: COM-RE), is selected to perform char gasification by using kinetic reactions. The gases released are purified by gas-solid separation.

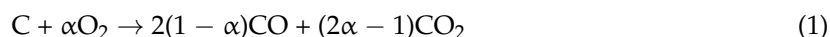
The operating condition is chosen based on the published data of the simulation of biomass gasification in a fluidized bed reactor using ASPEN PLUS by Nikoo & Mahinpey [14], as shown in Table 2.

**Table 2.** Parameter inputs in simulation study.

<b>Biomass Feedstock</b>		
Proximate analysis		
- Moisture	wt. %	8
- Volatile matter	wt. % dry basis	82.29
- Fixed carbon	wt. % dry basis	17.16
- Ash	wt. % dry basis	0.55
Ultimate analysis		
- C	wt. % dry basis	50.54
- H	wt. % dry basis	7.08
- O	wt. % dry basis	41.11
- N	wt. % dry basis	0.15
- S	wt. % dry basis	0.55
- Ash	wt. % dry basis	0.57
Flow rate	kg/h	0.445–0.512
<b>Air Feedstock</b>		
Temperature	°C	65
Flow rate	Nm <sup>3</sup> /h	0.5–0.7
<b>Steam Feedstock</b>		
Temperature	°C	145
Flow rate	kg/h	0–1.8
<b>Operating Condition</b>		
Temperature	°C	700–900
Pressure	atm	1

The operating temperature, pressure, reactor volume, and reaction information are identified in the reactor COM-RE. The production compositions are calculated with the assumption that the simulation is carried out with the power-law kinetics. The gas-film-diffusion-controlled regime of combustion reaction is selected for the input kinetic parameters. The stoichiometric reaction of the combustion zone and reduction zone are given in Equations (1) and (5).

Combustion reaction:



In the steam gasification system, the following two reactions could be assumed to take place.

Steam gasification reaction:



Equation (3) can be replaced by the following equation:



Equations (2) and (4) can be combined into the following equation



$\alpha$  is a mechanism factor which is experimentally varied between 0.5 and 1 for partial combustion reaction [24].  $\beta$  can be determined to be in the range of 1.1–1.5 when the operating temperature is in the range of 750–900 °C [25]. For this study, the values of  $\alpha$  and  $\beta$  are selected to obtain the best agreement with experimental data at 0.7 and 1.3, respectively. The reaction rate equations are defined as follows:

$$\frac{dX_1}{dt} = k_1 \exp\left(\frac{-E_1}{RT}\right) P_{O_2}^n (1 - X_1)^{\frac{2}{3}} \quad (6)$$

$$\frac{dX_2}{dt} = k_2 \exp\left(\frac{-E_2}{RT}\right) P_{H_2O}^n (1 - X_2)^{\frac{2}{3}} \quad (7)$$

The carbon conversion can be separately calculated with char combustion reaction as Equation (6) and char steam gasification reaction as Equation (7). For atmospheric gasification, the steam partial pressure is in the range of 0.25–0.8 atm, the parameter  $n$  can be equal to 1 according to the study by Kasaoka et al. [26]. The activation energies and reaction-rate constants of combustion reaction are dependent on the reaction control step, where  $k_1 = 75,785 \text{ s}^{-1} \cdot \text{atm}^{-1}$  and  $E_1/R = 13,523 \text{ K}$  for the chemical-reaction-controlled regime;  $k_1 = 0.44 \text{ s}^{-1} \cdot \text{atm}^{-1}$  and  $E_1/R = 3342.4 \text{ K}$  for the pore-diffusion-controlled regime; and  $k_1 = 0.046 \text{ s}^{-1} \cdot \text{atm}^{-1}$  and  $E_1/R = 1166 \text{ K}$  for the gas-film-diffusion-controlled regime;  $k_2 = 6474.7 \text{ s}^{-1} \cdot \text{atm}^{-1}$  and  $E_2/R = 19,544 \text{ K}$  for the steam gasification reaction [24].

### 2.3. Model Validation

The simulation models are validated with the experimental data and the work of Nikoo & Mahinpey [14] by calculating the root mean square error of synthesis gas compositions such as hydrogen, carbon dioxide, carbon monoxide, and methane. The root mean square error can be calculated according to below Equations (8) and (9).

$$\text{Mean Square Error (MSE)} = \frac{1}{N} \sum_{i=1}^N \left( \frac{y_{ie} - y_{ip}}{y_{ie}} \right)^2 \quad (8)$$

$$\text{Root Mean Square Error (RMSE)} = \sqrt{\text{MSE}} \quad (9)$$

where  $y_{ie}$  and  $y_{ip}$  are experimental and simulation compositions of synthesis gas composition ( $H_2$ ,  $CO$ ,  $CO_2$ , and  $CH_4$ ) respectively.

## 3. Results and Discussion

The simulation tests have been carried out in two parts. The first part is to validate the ASPEN Plus model with the experiment and the second part is to determine an energy self-sufficient condition with several sets of operating parameters.

### 3.1. Validation of the ASPEN Plus Model

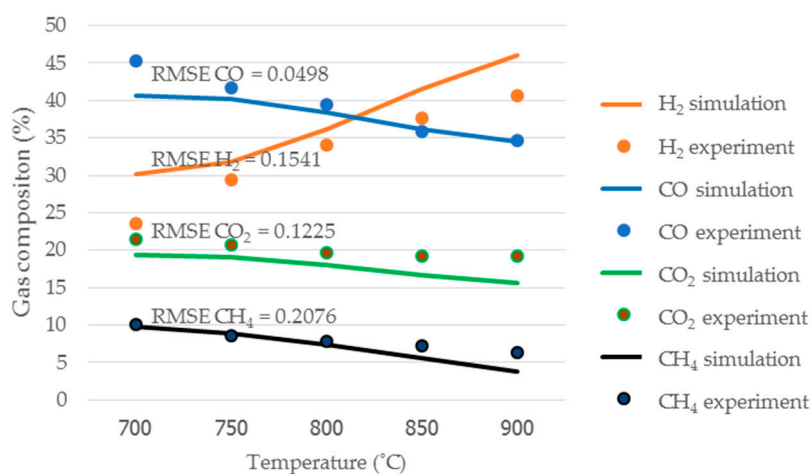
To perform the validation of the ASPEN Plus model with the work of Nikoo & Mahinpey [14], in this work, three variables: gasification temperature, equivalence ratio, and steam-to-biomass were considered and varied from 700–900 °C, 0.19 to 0.27, and 0 to 4.04 respectively.

#### 3.1.1. Validation of the ASPEN Plus model with Respect to Gasification Temperature

The validation of the effect on the gasification temperature varied from 700 °C to 900 °C on synthesis gas composition is shown in Figure 3. The RMSE of each component also given in the Figure 3 is less than 0.2076 which is better than that of Nikoo & Mahinpey [14]. It can be seen that



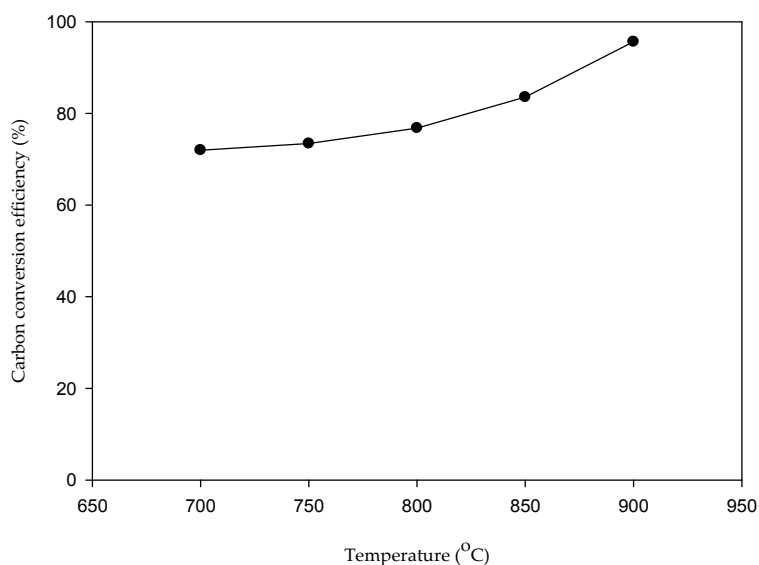
when the gasification temperature is increased, the composition of hydrogen increases while methane, carbon monoxide, and carbon dioxide decrease.



**Figure 3.** Experimental and simulation data comparison of gas composition with respect to gasification temperature.

In addition, the ASPEN Plus model can provide the gas composition with respect to type of reaction and reactor with good accuracy. H<sub>2</sub> is produced by the steam gasification reaction in the reactor COM-RE (RCSTR). CO is produced by both volatile reaction in the reactor VOLATILE (RGIBBS) and char combustion reaction in the reactor COM-RE (RCSTR), whereas CO<sub>2</sub> is only produced by char combustion reaction in the reactor COM-RE (RCSTR). Finally, CH<sub>4</sub> is only produced by volatile reaction in the reactor VOLATILE (RGIBBS) with Gibbs free energy equilibrium.

Figure 4 shows the carbon conversion efficiency with respect to gasification temperature based on the ASPEN Plus model. It can be seen that the carbon conversion efficiency increases when the gasification temperature increases because the reaction rate constant of char combustion reactions in the Arrhenius equation are directly proportional to temperature.



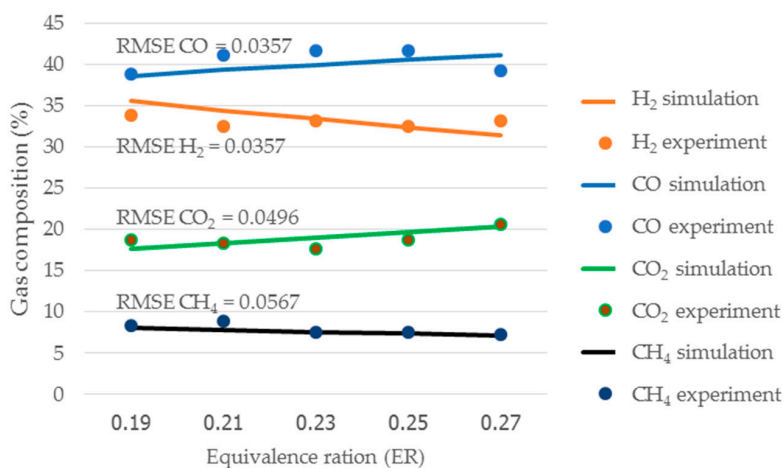
**Figure 4.** Carbon conversion efficiency with respect to temperature.



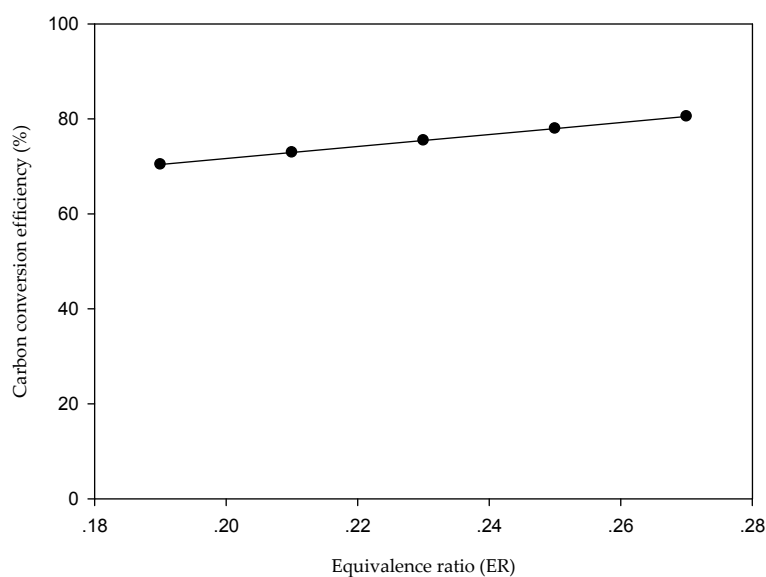
### 3.1.2. Validation of ASPEN Plus Model with Respect to Equivalence Ratio (ER)

The validation of the ASPEN Plus model by varying the equivalence ratio on gas composition is shown in Figure 5. The RMSE of each component also given in the Figure 5 is less than 0.0567 which is better than that of Nikoo & Mahinpey [14]. The increase in the equivalence ratio excites the reaction rate of the char combustion reaction in the RCSTR reactor. According to the stoichiometry of reaction in Equation (1),  $\text{CO}_2$  is produced more than CO with the same amount of oxygen gas, therefore the increase in the rate of  $\text{CO}_2$  is higher than the increase in the rate of CO. On the other hand,  $\text{CH}_4$  is not affected because the reaction rate of volatiles in the RGIBBS reactor and char gasification in the RCSTR reactor are not affected by the equivalence ratio.  $\text{H}_2$  concentration decreases with the increase in equivalence ratio due to the decrease in the reaction rate of char gasification.

As shown in Figure 6, the carbon conversion efficiency is also increased because the reaction rate of char combustion reaction is proportionally sensitive to the equivalence ratio. However, the carbon conversion efficiency can decrease when too much air is supplied. The biomass would be rapidly moved up to the gasifier before it would be completely reacted.



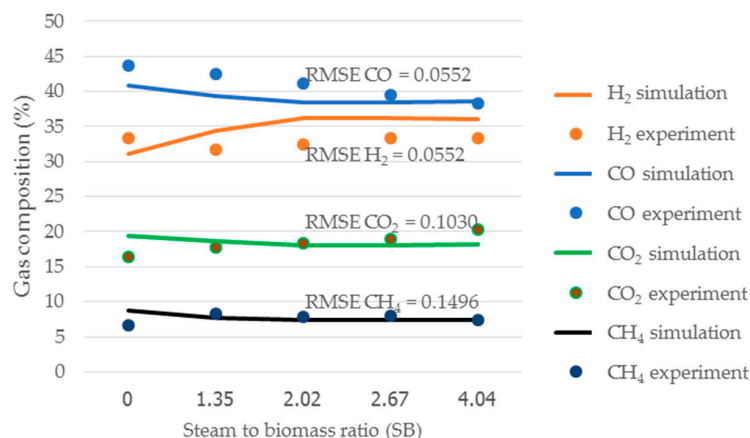
**Figure 5.** Experimental and simulation data comparison of gas composition with respect to equivalence ratio.



**Figure 6.** Carbon conversion efficiency with respect to equivalence ratio.

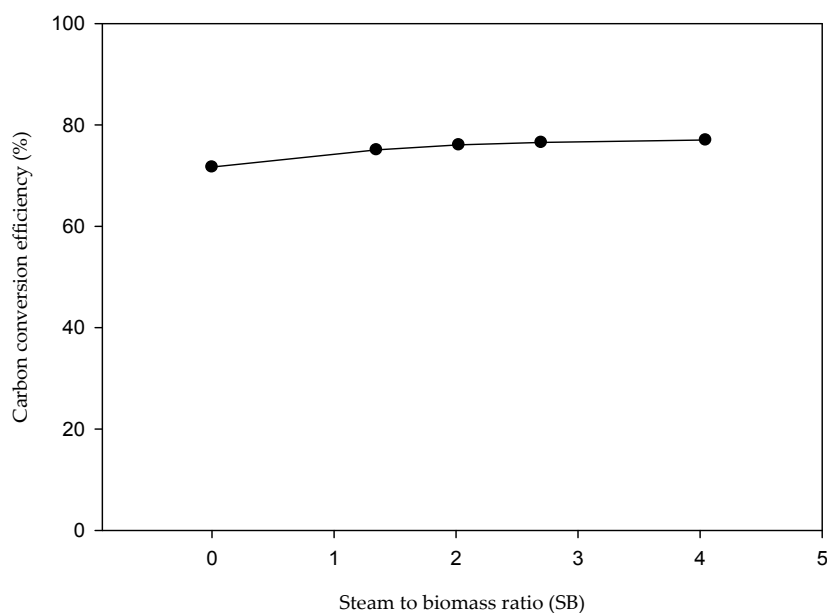
### 3.1.3. Validation of ASPEN Plus Model with Respect to Steam-to-Biomass Ratio (SB)

The validation of ASPEN Plus model by varying steam-to-biomass ratio in the range from 0 to 4.04 on synthesis gas composition is shown in Figure 7. The RMSE of each component also given in the Figure 7 is less than 0.1496 which is better than that of Nikoo & Mahinpey [14]. Refer to the stoichiometry of reaction in Equation (5),  $H_2$  concentration increases with increasing of reaction rate while the concentrations of CO and  $CO_2$  are not significantly affected because the reaction rate of char combustion is higher than the reaction rate of char gasification. For  $CH_4$ , there is no effect because the reaction rate of volatiles in the RGIBBS reactor and char gasification in the RCSTR reactor are not affected by steam-to-biomass ratio.



**Figure 7.** Experimental and simulation data comparison of gas composition with respect to steam-to-biomass ratio.

As shown in Figure 8, the carbon conversion efficiency increases when steam-to-biomass ratio increases due to the increase in reaction rate of char gasification reaction. However, the carbon conversion efficiency can be decreased in the case that steam is over-supplied, resulting in more moisture contained in the biomass which leads to obstruction of the combustion reaction of char.



**Figure 8.** Carbon conversion efficiency with respect to steam to biomass ratio.

### 3.1.4. Conclusion of ASPEN Plus Model Validation

The simulation model has been validated and compared with both experimental data and simulation results from Nikoo & Mahinpey [14]. The root mean square errors of all gas product compositions obtained from simulation are given in Table 3.

**Table 3.** The root mean square error of simulation results obtained from Nikoo & Mahinpey [14] and this work.

Set of Operating Condition	Result Source	Root Mean Square Error (RMSE)			
		H <sub>2</sub>	CO <sub>2</sub>	CO	CH <sub>4</sub>
Gas composition versus temperature	Nikoo & Mahinpey	0.3606	0.3009	0.1044	0.2152
	This work	0.1541	0.1225	0.0498	0.2076
% Reduction		<b>57.26</b>	<b>58.48</b>	<b>52.30</b>	<b>3.53</b>
Gas composition versus ER	Nikoo & Mahinpey	0.1981	0.2308	0.0939	0.1997
	This work	0.0357	0.0496	0.0357	0.0567
% Reduction		<b>81.99</b>	<b>78.51</b>	<b>61.98</b>	<b>71.61</b>
Gas composition versus SB ratio	Nikoo & Mahinpey	0.2045	0.2382	0.1143	0.2712
	This work	0.0552	0.1030	0.0552	0.1496
% Reduction		<b>73.01</b>	<b>56.76</b>	<b>51.71</b>	<b>44.84</b>

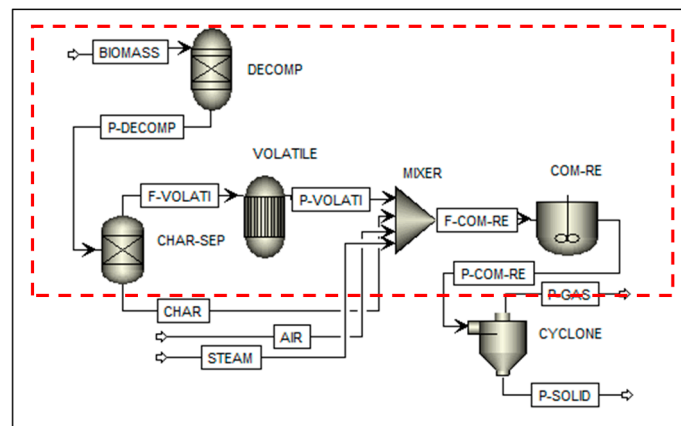
It is observed that the ASPEN Plus mode of this work is in good agreement with the experimental data and values of root mean square errors are less than the simulation results of Nikoo & Mahinpey in all cases [14].

### 3.2. Energy Self-Sufficient Condition

Simulation of the gasification to find out energy self-sufficient conditions is carried out according to variation of three input parameters: gasification temperature, equivalence ratio, and steam-to-biomass ratio. Sensitivity analysis was carried out to determine energy self-sufficient conditions. The equilibrium point of the energy self-sufficient process is the summation of the thermal energies from all reactions—heat source and heat sink—taking place inside the gasifier are zero as shown in Equation (10). The summation of the energy balance of all thermal reactors as shown in Figure 9.

$$Q_{\text{gasifier (net)}} = Q_{\text{decomp}} + Q_{\text{volatile}} + Q_{\text{com-re}} = 0 \quad (10)$$

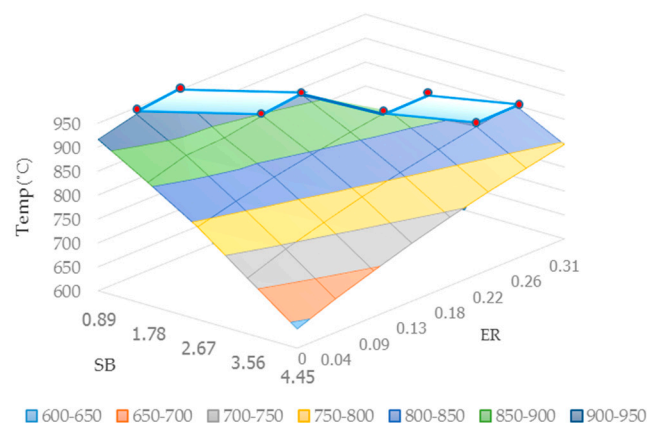
The variation of operating conditions has been carried out in order to find desired sets of the operating parameters; biomass was fed into the process at 0.445 kg/h, air supply flow rate was varied from 0 Nm<sup>3</sup>/h to 0.7 Nm<sup>3</sup>/h, or the equivalence ratio was varied from 0 to 0.31 and steam supply flow rate was varied from 0 to 2 kg/h, or the steam-to-biomass ratio was varied from 0 to 4.45. In each case, the equivalence ratio and steam-to-biomass ratio were fixed and the gasification temperature was varied to find the energy self-sufficient condition via the use of the ASPEN Plus simulator software. The trial and error of operating conditions has been selected as the technic in order to find the various sets of suitable operating parameter. According to Boerrigter and Rauch [27], the product distribution depended on the conditions in the gasification such as the gasification medium, gasifier design, residence time, etc. Greater amounts of carbon dioxide could decrease the heating value of synthesis gas [27]. Therefore, suitable criteria of gas composition to promote the heating value were the volumetric percentages of carbon dioxide and the carbon conversion efficiency which should be lower than 20% and more than 70% respectively.



**Figure 9.** The system of energy balance in the steam gasification process.

After completion of the simulation test, the energy self-sufficient conditions with respect to the gasification temperature, equivalence ratio, and steam-to-biomass ratio were plotted in 3D graph to exhibit the surface area as shown in Figure 10 and the simulation results of the energy self-sufficient conditions in the steam gasification process are listed in the Appendix A.

An equivalence ratio was varied from 0 to 0.31, and steam-to-biomass ratio was varied from 0 to 4.45. The gasification temperature was selected in a range of 600–1000 °C. The shaded regions show the areas where the carbon conversion efficiency is higher than 70% and carbon dioxide oxide gas is lower than 20 volumetric percentages. The optimum point of the simulation was found at gasification temperature of 911 °C, equivalence ratio of 0.18, and steam-to-biomass ratio of 1.78. This operating point gives the maximum of carbon conversion efficiency of 91.03%, and carbon dioxide oxide gas is still in the acceptable range at 15.18 volumetric percentages. However, if no steam is supplied, the energy self-sufficient condition cannot be achieved because there is not any endothermic energy produced by char gasification reaction to balance the exothermic energy which occurs in pyrolysis and combustion zones. In this study, the energy self-sufficient regions can be found when the steam-to-biomass ratio is between 0.89 and 3.56. If the steam-to-biomass ratio is above 3.56, meaning that large amount of steam is fed to the RCSTR reactor, the carbon conversion ratio would be less than 70% in any operating scenarios.



**Figure 10.** The relationship of key parameters for the energy self-sufficient condition.

### 3.3. Environmental Assessment

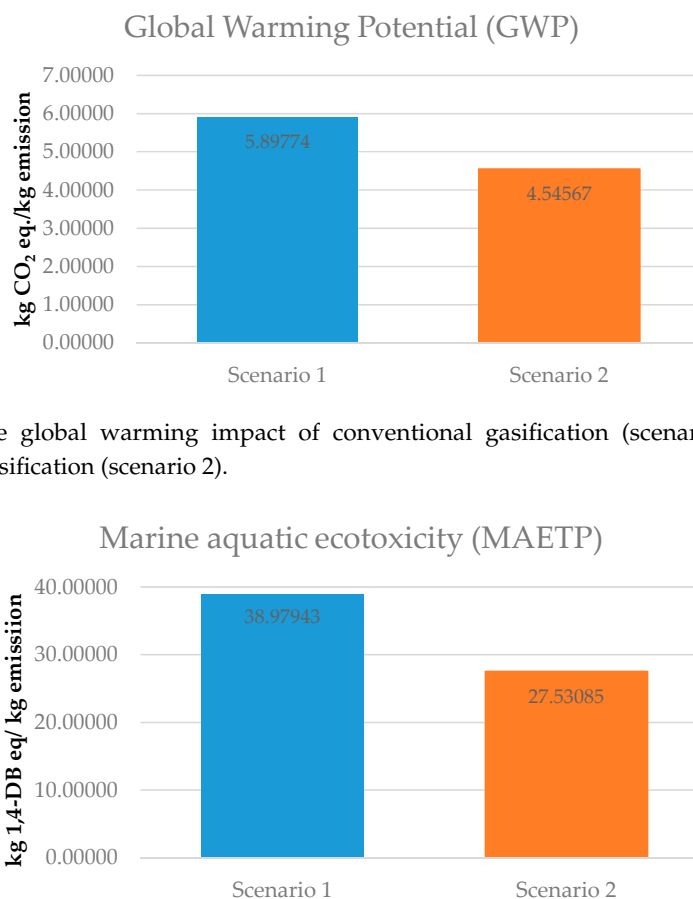
Life cycle assessment (LCA) is a useful tool to demonstrate different impact categories involved, quantitatively and qualitatively, throughout the life cycle of the end product [28]. It can also be used to

assess the environmental impacts of biomass gasification process by evaluating all CO<sub>2</sub> related inputs and outputs of the system [9]. Environmental analysis has been carried out using SimaPro software to evaluate in terms of environmental impacts. SimaPro (Version 7.3) with the CML 2 baseline 2000 methodology (the method which proposed by a group of scientists under the lead of CML (Center of Environmental Science of Leiden University)) was used to calculate the potential environmental impacts. Impact categories were selected which relate to gasification output. Ten impact potentials are evaluated: abiotic depletion (ADP), acidification (AP), eutrophication (EP), global warming (GWP), ozone layer depletion (ODP), human toxicity (HTP), fresh-water aquatic ecotoxicity (FAETP), marine aquatic ecotoxicity (MAETP), terrestrial ecotoxicity (TETP), and photochemical oxidation (POFP). However, two more impacted categories are the marine aquatic ecotoxicity and global warming.

Marine aquatic ecotoxicity refers to impacts of toxic substances on marine ecosystems. Characterization factors are expressed as 1,4-dichlorobenzene equivalents/kg emission. For global warming, the reference substance is CO<sub>2</sub>. All greenhouse gases are expressed in the units of kg CO<sub>2</sub> equivalents/kg emission.

Environmental analysis is performed to compare two scenarios: conventional gasification (scenario 1) and energy self-sufficient gasification (scenario 2).

Figures 11 and 12 show the environmental impacts: global warming potential and marine aquatic ecotoxicity respectively of the two scenarios. It is apparent that the energy self-sufficient gasification produces lower environmental impacts (GWP and MAETP) than conventional gasification does.



**Figure 11.** The global warming impact of conventional gasification (scenario 1) and energy self-sufficient gasification (scenario 2).

**Figure 12.** The marine aquatic ecotoxicity impact of conventional gasification (scenario 1) and energy self-sufficient gasification (scenario 2).

#### 4. Conclusions

In this study, the thermodynamic equilibrium analysis of a steam gasification process from biomass has been carried out by representing of the gasification reactor with three sequencing reactors (RYIELD reactor, RGIBBS reactor, and RCSTR reactor) in the ASPEN Plus simulator software. In this work, the biomass used was pine sawdust and the biomass gasification technology was fluidized bed technology (conventional gasification). The effect of three operating parameters (gasification temperature, equivalence ratio, and steam-to-biomass ratio) were analyzed and compared with the experimental data and the work of Nikoo & Mahinpey [14]. Then, energy self-sufficient conditions were achieved when gasification temperature, equivalence ratio, and steam-to-biomass ratio were properly selected.

Simulation results show that the unit operation blocks, including separation processes and many types of reactors in process simulation model by ASPEN Plus give good agreement with the experimental data and more accurate than the work of Nikoo & Mahinpey [14]. Furthermore, the increase in temperature and steam-to-biomass ratio can improve the steam gasification process. Hydrogen and carbon conversion efficiencies increase but carbon dioxide, carbon monoxide, and methane efficiencies decrease. In addition, the increase in equivalence ratio gives more carbon dioxide, carbon monoxide, and carbon conversion efficiency. However, the complete combustion needed to be avoided in order to limit the volumetric percentage of carbon dioxide in the synthesis gas.

The simulation study was run to find the relationship among gasification temperature, equivalence ratio, and steam-to-biomass ratio to obtain the energy self-sufficient condition. The equivalence ratio was varied from 0 to 0.31 and the steam-to-biomass ratio was varied from 0 to 4.45. The gasification temperature was selected from a range of 600–1000 °C. Finally, the optimum condition was found at a gasification temperature of 911 °C, equivalence ratio of 0.18, and steam-to-biomass ratio of 1.78. This operating point gave the maximum of carbon conversion efficiency at 91.03%, and carbon dioxide oxide gas was still in criteria at 15.18 volumetric percentages.

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**Author Contributions:** Ajaree Suwatthikul and Siripong Limprachaya developed and validated the model and determined energy self-sufficient conditions. Ajaree Suwatthikul and Paisan Kittisupakorn carried out LCA simulation and analysis. Ajaree Suwatthikul and Paisan Kittisupakorn contributed to writing and reviewing the manuscript. Paisan Kittisupakorn and Iqbal Mohammed Muftaba supervised the whole work.

**Conflicts of Interest:** The authors declare no conflict of interest.

#### Appendix A

**Table A1.** The simulation results of the energy self-sufficient conditions in the steam gasification process.

ER	SB	Temperature (°C)	Gas Composition (vol. %)				Carbon Conversion (%)
			H <sub>2</sub>	CO	CO <sub>2</sub>	CH <sub>4</sub>	
0	0.89	916	56.34	28.89	10.24	4.53	62.80
0.04	0.89	936	53.82	30.51	11.76	3.91	76.81
0.09	0.89	949	51.36	31.91	13.23	3.50	90.34
0	1.78	856	55.68	28.50	8.86	6.96	41.55
0.04	1.78	880	52.68	30.61	11.32	5.39	57.49
0.09	1.78	884	48.92	32.66	13.63	4.79	69.57
0.13	1.78	898	48.72	32.99	13.91	4.38	76.33
0.18	1.78	911	46.99	34.05	15.18	3.78	91.30
0	2.67	793	56.12	26.60	5.80	11.48	25.12
0.04	2.67	814	51.58	29.76	9.74	8.93	35.27

Table A1. Cont.

ER	SB	Temperature (°C)	Gas Composition (vol. %)				Carbon Conversion (%)
			H <sub>2</sub>	CO	CO <sub>2</sub>	CH <sub>4</sub>	
0.09	2.67	832	48.58	31.92	12.22	7.29	45.89
0.13	2.67	847	43.92	34.88	15.38	5.81	62.80
0.18	2.67	861	44.87	34.58	15.24	5.31	67.63
0.22	2.67	873	43.73	35.40	16.19	4.69	78.26
0.26	2.67	832	42.74	36.10	16.98	4.18	89.37
0	3.56	716	54.96	25.24	2.14	17.67	16.43
0.04	3.56	744	48.15	30.10	8.21	13.54	24.64
0.09	3.56	767	43.77	33.35	11.94	10.94	33.33
0.13	3.56	788	44.63	33.15	12.17	10.04	35.75
0.18	3.56	806	40.20	36.13	16.14	7.54	51.69
0.22	3.56	822	37.91	37.91	17.63	6.56	61.84
0.26	3.56	837	37.75	38.29	18.30	5.66	71.50
0.31	3.56	850	37.59	38.54	18.90	4.98	81.64
0	4.45	640	54.85	24.16	0.42	20.57	14.49
0.04	4.45	670	45.04	30.56	7.51	16.89	21.26
0.09	4.45	696	41.84	33.30	11.41	13.45	28.02
0.13	4.45	721	36.27	37.01	15.07	11.66	35.27
0.18	4.45	743	34.98	38.10	17.09	9.84	43.00
0.22	4.45	763	33.79	39.16	18.60	8.45	51.21
0.26	4.45	780	32.83	40.09	19.70	7.39	59.42
0.31	4.45	797	31.90	41.01	20.56	6.52	68.12

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